Bis(4-benzylpiperidine-1-carbodithioato-kappa S-2,S ')-dimethyltin(IV)

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Bis(4-benzylpiperidine-1-carbodithioato-κ^2S,S')-dimethyltin(IV)

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.003 Å
R factor = 0.020
wR factor = 0.051
Data-to-parameter ratio = 14.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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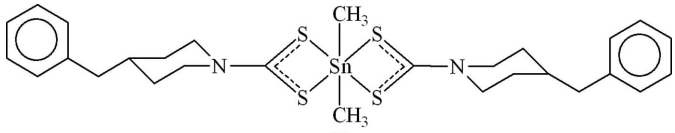
The Sn atom in the title compound, $[Sn(CH_3)_2(C_{13}H_{16}NS_2)_2]$, has a highly distorted octahedral geometry that may be best described as skew-trapezoidal planar for thiocarboxylates. The ligands are asymmetrically coordinated to the Sn atom, with shorter Sn—S bond lengths that are very close to the sum of the covalent radii of Sn and S, while the longer Sn—S distances are significantly less than the sum of their van der Waals radii.

Comment

The increasing industrial use of organotin(IV) compounds containing an Sn—S bond, especially as stabilizers of polyvinyl chlorides (Tarassoli *et al.*, 2006), and the recognition of the importance of this bond for the biological properties of organotin compounds (Barbieri *et al.*, 1989), have together spurred the study of thiolates (Casas *et al.*, 1997, 1999). We present here the crystal structure of the title compound, (I).



(I)

The structure of (I) is composed of a discrete monomeric molecule (Fig. 1), in which the Sn atom exists in a skew–trapezoidal planar geometry. The equatorial plane is defined by four S atoms from two chelating thiocarboxylate ligands. The Sn atom is 0.016 (1) Å out of the least-squares plane formed by the four S atoms, and on the same side as atom C28. The two remaining octahedral sites are occupied by two methyl groups which lie over the weaker Sn—S bonds and define a C27—Sn—C28 angle of 135.64 (7)°. The angle between the Sn—C27 bond and the least-squares plane is 69.92 (5)°, and that between the Sn—C28 bond and the least-squares plane is 65.71 (5)°.

The degrees of asymmetry in the modes of coordination of each thiocarboxylate ligand, while comparable, are not equivalent. The first ligand forms Sn—S1 and Sn—S2 bond distances of 2.5190 (4) and 2.9779 (5) Å, respectively, while the other forms Sn—S3 and Sn—S4 bonds of 2.5240 (4) and 2.9715 (4) Å, respectively; the shorter bond lengths are close to the sum of the covalent radii of Sn and S and the longer distances are significantly less than the sum of their van der Waals radii (4.0 Å) (Ma *et al.*, 2003).

The C—S bond distances [S1—C13 = 1.7548 (16) Å and S3—C26 = 1.7496 (16) Å] for the S atoms bound strongly to the Sn centre are longer than the C—S bonds [S2—C13 =

1.6902 (16) Å and S4—C26 = 1.6990 (15) Å] involving the S atoms forming the weaker bonds to the Sn atom. The geometry of complex (I) is similar to those usually observed for $R_2Sn(S_2CNR'_2)$ compounds (Tiekink, 1992, 1993).

Experimental

To a solution of 4-benzylpiperidine-1-carbodithioic acid (0.5 g, 1.99 mmol) in dry methanol (40 ml), a solution of dimethyltin(IV) chloride (0.218 g, 0.995 mmol) in methanol (40 ml) was added dropwise and the mixture was stirred vigorously for 3 h. The resulting white solid was separated off and the filtrate was allowed to evaporate to obtain white crystals.

Crystal data

$[Sn(CH_3)_2(C_{13}H_{16}NS_2)_2]$	V = 1480.99 (15) Å^3
M_r = 649.60	Z = 2
Triclinic, $P\overline{1}$	D_x = 1.457 Mg m^{-3}
a = 9.8937 (6) Å	Mo $K\alpha$ radiation
b = 11.4658 (7) Å	μ = 1.16 mm^{-1}
c = 14.2179 (8) Å	T = 100 (1) K
α = 99.811 (1)°	Block, colourless
β = 108.859 (1)°	0.49 × 0.43 × 0.41 mm
γ = 96.158 (1)°	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	11332 measured reflections 6972 independent reflections
φ and ω scans	6620 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)	R_{int} = 0.013
T_{min} = 0.540, T_{max} = 0.620	θ_{max} = 28.3°

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0252P)^2 + 0.4409P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.020	
$wR(F^2)$ = 0.051	
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.001
6972 reflections	$\Delta\rho_{max}$ = 0.53 e Å^{-3}
468 parameters	$\Delta\rho_{min}$ = −0.43 e Å^{-3}
All H-atom parameters refined	

All H atoms were located in a difference Fourier map and refined isotropically.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2000); data reduction: *XPREP* (Bruker, 2000); program(s) used to solve structure: *DIRDIF99* (Beurskens *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

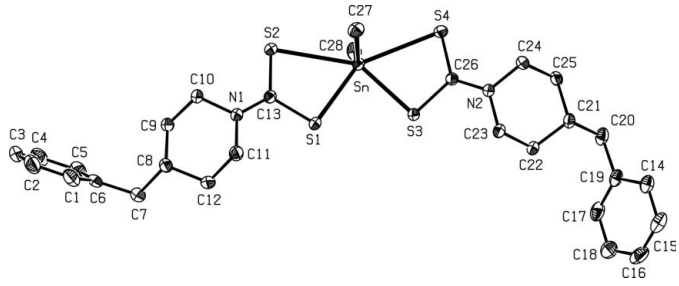


Figure 1
A perspective drawing of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.

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Crystal data

$[Sn(CH_3)_2(C_{13}H_{16}NS_2)_2]$
$M_r = 649.60$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.8937$ (6) Å
$b = 11.4658$ (7) Å
$c = 14.2179$ (8) Å
$\alpha = 99.811$ (1)°
$\beta = 108.859$ (1)°
$\gamma = 96.158$ (1)°
$V = 1480.99$ (15) Å^3
$Z = 2$
$F(000) = 668$
The final unit cell was obtained from the xyz centroids of 9452 reflections after integration using the SAINTPLUS software package (Bruker, 2000).
Reduced cell calculations did not indicate any higher metric lattice symmetry and examination of the final atomic coordinates of the structure did not yield extra symmetry elements (Spek, 1988; Le Page 1987, 1988)
$D_x = 1.457$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9452 reflections
$\theta = 2.7$–$29.8°$
$\mu = 1.16$ mm^{-1}
$T = 100$ K
Block, colourless
0.49 × 0.43 × 0.41 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine focus sealed Siemens Mo tube
Parallel mounted graphite monochromator
Detector resolution: 4096x4096 / 62x62 (binned 512) pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)
$T_{min} = 0.540$, $T_{max} = 0.620$
11332 measured reflections
6972 independent reflections
6620 reflections with $I > 2\sigma(I)$
$R_{int} = 0.013$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.6°$
$h = -13 \rightarrow 12$
$k = -15 \rightarrow 15$
$l = -18 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.020$
$wR(F^2) = 0.051$
$S = 1.04$
6972 reflections
468 parameters
0 restraints
Primary atom site location: heavy-atom method
Secondary atom site location: structure-invariant direct methods
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0252P)^2 + 0.4409P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.53$ e Å^{-3}
$\Delta\rho_{min} = -0.43$ e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn	0.99487 (1)	0.37860 (1)	0.22505 (1)	0.0172 (1)
S1	0.77165 (4)	0.21795 (3)	0.15723 (3)	0.0208 (1)
S2	0.71626 (4)	0.46280 (3)	0.13579 (3)	0.0249 (1)
S3	1.12035 (4)	0.20196 (3)	0.25974 (3)	0.0224 (1)
S4	1.31412 (4)	0.43929 (3)	0.33146 (3)	0.0244 (1)
N1	0.50847 (14)	0.27619 (11)	0.10107 (10)	0.0213 (4)
N2	1.39441 (14)	0.23714 (11)	0.38351 (10)	0.0206 (4)
C1	−0.1280 (2)	0.16235 (17)	−0.11731 (15)	0.0343 (5)
C2	−0.2443 (2)	0.22060 (18)	−0.15226 (16)	0.0388 (6)
C3	−0.2627 (2)	0.26715 (17)	−0.23819 (16)	0.0371 (6)
C4	−0.1645 (2)	0.25586 (18)	−0.28764 (15)	0.0373 (6)
C5	−0.0483 (2)	0.19899 (16)	−0.25189 (14)	0.0333 (5)
C6	−0.02758 (19)	0.15082 (14)	−0.16629 (13)	0.0283 (5)
C7	0.1006 (2)	0.08967 (15)	−0.12647 (15)	0.0316 (5)
C8	0.21326 (17)	0.15897 (13)	−0.02499 (12)	0.0230 (4)
C9	0.27774 (18)	0.28381 (13)	−0.02975 (12)	0.0222 (4)
C10	0.39554 (18)	0.34990 (14)	0.06970 (13)	0.0239 (4)
C11	0.44982 (19)	0.15745 (14)	0.11080 (13)	0.0260 (5)
C12	0.33564 (19)	0.08891 (14)	0.01134 (14)	0.0269 (5)
C13	0.64974 (16)	0.31800 (12)	0.12792 (11)	0.0183 (4)
C14	1.83150 (19)	−0.11115 (16)	0.46298 (14)	0.0277 (5)
C15	1.8220 (2)	−0.23309 (17)	0.46302 (16)	0.0350 (6)
C16	1.7315 (2)	−0.31705 (17)	0.37774 (18)	0.0401 (7)
C17	1.6531 (2)	−0.28004 (18)	0.29222 (17)	0.0389 (6)
C18	1.6634 (2)	−0.15865 (17)	0.29220 (14)	0.0322 (6)
C19	1.75187 (18)	−0.07210 (14)	0.37761 (13)	0.0247 (5)
C20	1.75657 (19)	0.05982 (16)	0.37874 (14)	0.0276 (5)
C21	1.64333 (17)	0.11384 (13)	0.41763 (12)	0.0209 (4)
C22	1.48909 (17)	0.04880 (13)	0.35580 (12)	0.0207 (4)
C23	1.37638 (18)	0.10892 (14)	0.38764 (13)	0.0232 (5)
C24	1.53928 (18)	0.30319 (14)	0.44885 (13)	0.0245 (4)
C25	1.65449 (17)	0.24772 (14)	0.41645 (13)	0.0237 (4)
C26	1.28996 (16)	0.29037 (12)	0.33160 (11)	0.0186 (4)
C27	0.9874 (2)	0.46719 (15)	0.36686 (13)	0.0269 (5)
C28	1.0364 (2)	0.43318 (17)	0.10113 (13)	0.0278 (5)
H1	−0.112 (2)	0.1323 (19)	−0.0585 (17)	0.039 (6)*

H2	−0.308 (3)	0.229 (2)	−0.1181 (17)	0.043 (6)*
H3	−0.341 (3)	0.308 (2)	−0.2630 (17)	0.043 (6)*
H4	−0.175 (3)	0.290 (2)	−0.3419 (19)	0.052 (7)*
H5	0.017 (2)	0.188 (2)	−0.2891 (17)	0.043 (6)*
H7	0.153 (2)	0.0776 (19)	−0.1764 (16)	0.042 (6)*
H7′	0.065 (3)	0.015 (2)	−0.1152 (18)	0.051 (7)*
H8	0.166 (2)	0.1691 (16)	0.0247 (14)	0.024 (5)*
H9	0.322 (2)	0.2789 (17)	−0.0821 (15)	0.028 (5)*
H9′	0.204 (2)	0.3306 (17)	−0.0463 (14)	0.027 (5)*
H10	0.441 (2)	0.4260 (17)	0.0619 (14)	0.026 (5)*
H10′	0.354 (2)	0.3677 (17)	0.1262 (15)	0.032 (5)*
H11	0.402 (2)	0.1710 (18)	0.1646 (16)	0.036 (5)*
H11′	0.532 (2)	0.1116 (17)	0.1305 (15)	0.028 (5)*
H12	0.300 (2)	0.0123 (19)	0.0197 (16)	0.036 (5)*
H12′	0.386 (2)	0.0798 (19)	−0.0382 (16)	0.040 (6)*
H14	1.891 (2)	−0.0538 (18)	0.5221 (16)	0.031 (5)*
H15	1.875 (2)	−0.2537 (19)	0.5221 (16)	0.035 (5)*
H16	1.723 (3)	−0.399 (2)	0.3776 (18)	0.051 (7)*
H17	1.591 (3)	−0.339 (2)	0.232 (2)	0.057 (7)*
H18	1.612 (2)	−0.134 (2)	0.2356 (17)	0.040 (6)*
H20	1.852 (2)	0.1030 (18)	0.4199 (15)	0.030 (5)*
H20′	1.740 (2)	0.0743 (18)	0.3089 (16)	0.034 (5)*
H21	1.663 (2)	0.1065 (16)	0.4870 (15)	0.026 (5)*
H22	1.4760 (19)	−0.0322 (16)	0.3643 (13)	0.020 (4)*
H22′	1.470 (2)	0.0469 (16)	0.2849 (15)	0.025 (5)*
H23	1.283 (2)	0.0707 (16)	0.3448 (14)	0.024 (5)*
H23′	1.389 (2)	0.1089 (18)	0.4584 (16)	0.032 (5)*
H24	1.552 (2)	0.2982 (16)	0.5173 (15)	0.027 (5)*
H24′	1.546 (2)	0.3837 (17)	0.4449 (14)	0.025 (5)*
H25	1.751 (2)	0.2927 (18)	0.4613 (15)	0.030 (5)*
H25′	1.642 (2)	0.2583 (17)	0.3501 (15)	0.026 (5)*
H27	0.898 (3)	0.440 (2)	0.3682 (18)	0.048 (6)*
H27′	0.991 (2)	0.548 (2)	0.3659 (16)	0.037 (5)*
H27"	1.068 (3)	0.457 (2)	0.4165 (18)	0.047 (6)*
H28	0.962 (3)	0.402 (2)	0.0431 (18)	0.039 (6)*
H28′	1.046 (3)	0.516 (2)	0.1152 (18)	0.051 (7)*
H28"	1.118 (3)	0.412 (2)	0.099 (2)	0.062 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn	0.0186 (1)	0.0174 (1)	0.0154 (1)	0.0050 (1)	0.0052 (1)	0.0033 (1)
S1	0.0185 (2)	0.0176 (2)	0.0260 (2)	0.0057 (1)	0.0057 (2)	0.0063 (1)
S2	0.0196 (2)	0.0162 (2)	0.0357 (2)	0.0043 (1)	0.0050 (2)	0.0060 (2)
S3	0.0180 (2)	0.0176 (2)	0.0251 (2)	0.0046 (1)	0.0004 (1)	0.0007 (1)
S4	0.0248 (2)	0.0167 (2)	0.0262 (2)	0.0040 (1)	0.0019 (2)	0.0034 (1)
N1	0.0182 (6)	0.0188 (6)	0.0254 (7)	0.0042 (5)	0.0043 (5)	0.0066 (5)
N2	0.0170 (6)	0.0181 (6)	0.0235 (7)	0.0044 (5)	0.0031 (5)	0.0030 (5)

C1	0.0273 (9)	0.0372 (9)	0.0303 (9)	−0.0049 (7)	0.0022 (7)	0.0080 (7)
C2	0.0234 (10)	0.0446 (10)	0.0426 (11)	−0.0006 (8)	0.0098 (8)	0.0014 (8)
C3	0.0217 (9)	0.0298 (9)	0.0477 (12)	0.0024 (7)	−0.0017 (8)	0.0051 (8)
C4	0.0310 (10)	0.0396 (10)	0.0303 (10)	−0.0037 (8)	−0.0015 (8)	0.0093 (8)
C5	0.0270 (9)	0.0381 (9)	0.0268 (9)	0.0003 (7)	0.0043 (7)	−0.0006 (7)
C6	0.0226 (8)	0.0211 (7)	0.0291 (9)	−0.0025 (6)	−0.0013 (7)	−0.0021 (6)
C7	0.0266 (9)	0.0245 (8)	0.0334 (10)	0.0022 (7)	0.0009 (7)	−0.0001 (7)
C8	0.0194 (8)	0.0225 (7)	0.0240 (8)	0.0020 (6)	0.0039 (6)	0.0055 (6)
C9	0.0207 (8)	0.0206 (7)	0.0224 (8)	0.0042 (6)	0.0034 (6)	0.0047 (6)
C10	0.0188 (8)	0.0212 (7)	0.0271 (8)	0.0057 (6)	0.0024 (6)	0.0030 (6)
C11	0.0236 (8)	0.0248 (7)	0.0299 (9)	0.0041 (6)	0.0071 (7)	0.0116 (6)
C12	0.0252 (9)	0.0175 (7)	0.0335 (9)	0.0023 (6)	0.0048 (7)	0.0057 (6)
C13	0.0200 (7)	0.0188 (6)	0.0150 (7)	0.0055 (5)	0.0044 (5)	0.0032 (5)
C14	0.0259 (9)	0.0346 (9)	0.0288 (9)	0.0123 (7)	0.0132 (7)	0.0115 (7)
C15	0.0401 (11)	0.0413 (10)	0.0393 (10)	0.0237 (8)	0.0233 (9)	0.0212 (8)
C16	0.0445 (12)	0.0294 (9)	0.0610 (13)	0.0186 (8)	0.0324 (11)	0.0127 (9)
C17	0.0335 (10)	0.0360 (9)	0.0462 (12)	0.0131 (8)	0.0168 (9)	−0.0036 (8)
C18	0.0299 (10)	0.0417 (10)	0.0294 (9)	0.0186 (8)	0.0130 (8)	0.0064 (7)
C19	0.0225 (8)	0.0312 (8)	0.0291 (8)	0.0128 (6)	0.0157 (7)	0.0112 (6)
C20	0.0212 (8)	0.0337 (8)	0.0354 (9)	0.0106 (7)	0.0138 (7)	0.0156 (7)
C21	0.0169 (7)	0.0243 (7)	0.0224 (8)	0.0061 (5)	0.0054 (6)	0.0086 (6)
C22	0.0192 (8)	0.0202 (7)	0.0230 (8)	0.0063 (5)	0.0058 (6)	0.0065 (5)
C23	0.0187 (8)	0.0207 (7)	0.0306 (9)	0.0063 (6)	0.0073 (7)	0.0077 (6)
C24	0.0199 (8)	0.0209 (7)	0.0253 (8)	0.0028 (6)	0.0002 (6)	0.0010 (6)
C25	0.0174 (8)	0.0234 (7)	0.0259 (8)	0.0017 (6)	0.0016 (6)	0.0071 (6)
C26	0.0186 (7)	0.0182 (6)	0.0169 (7)	0.0045 (5)	0.0048 (5)	0.0005 (5)
C27	0.0326 (10)	0.0267 (8)	0.0228 (8)	0.0089 (7)	0.0120 (7)	0.0024 (6)
C28	0.0249 (9)	0.0395 (10)	0.0204 (8)	0.0064 (7)	0.0073 (7)	0.0112 (7)

Geometric parameters (Å, º)

Sn—S1	2.5190 (4)	C24—C25	1.520 (3)
Sn—S2	2.9779 (5)	C1—H1	0.93 (2)
Sn—S3	2.5240 (4)	C2—H2	0.92 (3)
Sn—S4	2.9715 (5)	C3—H3	0.95 (3)
Sn—C27	2.1253 (18)	C4—H4	0.91 (2)
Sn—C28	2.1103 (19)	C5—H5	0.96 (2)
S1—C13	1.7548 (16)	C7—H7	1.01 (2)
S2—C13	1.6902 (15)	C7—H7′	0.95 (2)
S3—C26	1.7496 (16)	C8—H8	0.96 (2)
S4—C26	1.6990 (15)	C9—H9	0.98 (2)
N1—C10	1.473 (2)	C9—H9′	0.94 (2)
N1—C11	1.468 (2)	C10—H10	0.98 (2)
N1—C13	1.333 (2)	C10—H10′	1.02 (2)
N2—C23	1.475 (2)	C11—H11	1.02 (2)
N2—C24	1.469 (2)	C11—H11′	1.01 (2)
N2—C26	1.335 (2)	C12—H12	0.95 (2)
C1—C2	1.388 (3)	C12—H12′	0.98 (2)

C1—C6	1.391 (3)	C14—H14	0.95 (2)
C2—C3	1.382 (3)	C15—H15	0.92 (2)
C3—C4	1.376 (3)	C16—H16	0.93 (2)
C4—C5	1.379 (3)	C17—H17	0.97 (3)
C5—C6	1.386 (3)	C18—H18	0.91 (2)
C6—C7	1.511 (3)	C20—H20	0.96 (2)
C7—C8	1.528 (3)	C20—H20′	1.00 (2)
C8—C9	1.525 (2)	C21—H21	0.96 (2)
C8—C12	1.524 (3)	C22—H22	0.957 (19)
C9—C10	1.521 (2)	C22—H22′	0.96 (2)
C11—C12	1.514 (3)	C23—H23	0.94 (2)
C14—C15	1.391 (3)	C23—H23′	0.97 (2)
C14—C19	1.392 (3)	C24—H24	0.95 (2)
C15—C16	1.384 (3)	C24—H24′	0.93 (2)
C16—C17	1.377 (3)	C25—H25	0.99 (2)
C17—C18	1.385 (3)	C25—H25′	0.94 (2)
C18—C19	1.393 (3)	C27—H27	0.91 (3)
C19—C20	1.506 (2)	C27—H27′	0.93 (2)
C20—C21	1.542 (3)	C27—H27"	0.91 (3)
C21—C22	1.524 (2)	C28—H28	0.90 (3)
C21—C25	1.531 (2)	C28—H28′	0.92 (2)
C22—C23	1.519 (3)	C28—H28"	0.88 (3)

S1···S2	2.9645 (5)	H5···H7	2.38 (3)
S1···S3	3.3221 (6)	H7···H5	2.38 (3)
S1···C27	3.6445 (18)	H7···H9	2.57 (3)
S2···S1	2.9645 (5)	H7···H12′	2.49 (3)
S2···C17^{i}	3.618 (2)	H7···C18^{xi}	2.99 (2)
S2···C9^{ii}	3.4973 (16)	H7′···H1	2.56 (4)
S2···C28	3.402 (2)	H7′···H12	2.50 (3)
S2···C27	3.4942 (18)	H7′···S3^{iii}	2.94 (2)
S3···C7^{iii}	3.6256 (19)	H8···C1	2.94 (2)
S3···S1	3.3221 (6)	H8···H1	2.57 (3)
S3···S4	2.9650 (6)	H8···H11	2.53 (3)
S4···C24^{iv}	3.6862 (17)	H9···H7	2.57 (3)
S4···C28	3.5132 (19)	H9···H12′	2.56 (3)
S4···S3	2.9650 (6)	H9···C17^{xi}	3.08 (2)
S4···C27	3.468 (2)	H9′···C6	2.77 (2)
S1···H20′^{v}	3.00 (2)	H9′···H28"^{v}	2.55 (3)
S1···H12^{iii}	3.16 (2)	H9′···S2^{ii}	3.02 (2)
S1···H11′	2.43 (2)	H10···S2	2.54 (2)
S2···H17^{i}	3.04 (3)	H10′···S4^{v}	3.06 (2)
S2···H10	2.54 (2)	H10′···H11	2.47 (3)
S2···H9′^{ii}	3.02 (2)	H10′···H28"^{v}	2.37 (4)
S3···H23	2.490 (19)	H11···H8	2.53 (3)
S3···H15^{vi}	3.04 (2)	H11···H10′	2.47 (3)
S3···H7′^{iii}	2.94 (2)	H11···H22′^{v}	2.39 (3)
S4···H10′^{vii}	3.06 (2)	H11′···S1	2.43 (2)

S4···H27"	3.06 (3)	H12···H7′	2.50 (3)
S4···H28"	3.19 (3)	H12···S1^{iii}	3.16 (2)
S4···H24′	2.56 (2)	H12′···H7	2.49 (3)
C7···S3^{iii}	3.6256 (19)	H12′···H9	2.56 (3)
C9···S2^{ii}	3.4973 (16)	H14···H20	2.48 (3)
C14···C23^{vi}	3.400 (3)	H14···C14^{x}	3.09 (2)
C15···C23^{vi}	3.557 (3)	H14···H20^{x}	2.56 (3)
C15···C26^{vi}	3.574 (3)	H15···S3^{vi}	3.04 (2)
C17···S2^{viii}	3.618 (2)	H15···C26^{vi}	3.08 (2)
C18···C22	3.257 (3)	H17···S2^{viii}	3.04 (3)
C22···C18	3.257 (3)	H18···C22	3.08 (2)
C23···C14^{vi}	3.400 (3)	H18···H20′	2.46 (3)
C23···C15^{vi}	3.557 (3)	H20···H14	2.48 (3)
C24···S4^{iv}	3.6862 (17)	H20···H25	2.55 (3)
C26···C15^{vi}	3.574 (3)	H20···C14^{x}	3.02 (2)
C27···S2	3.4942 (18)	H20···H14^{x}	2.56 (3)
C27···S4	3.468 (2)	H20′···S1^{vii}	3.00 (2)
C27···S1	3.6445 (18)	H20′···H18	2.46 (3)
C28···C28^{ix}	3.396 (3)	H20′···H22′	2.56 (3)
C28···S4	3.5132 (19)	H20′···H25′	2.47 (3)
C28···S2	3.402 (2)	H21···H24	2.59 (3)
C1···H28^{v}	3.09 (2)	H22···C18	2.809 (19)
C1···H8	2.94 (2)	H22···C19	2.77 (2)
C3···H28′^{ii}	2.96 (3)	H22′···C11^{vii}	2.929 (19)
C4···H28′^{ii}	3.09 (2)	H22′···H11^{vii}	2.39 (3)
C6···H9′	2.77 (2)	H22′···H20′	2.56 (3)
C8···H1	3.07 (2)	H23···S3	2.490 (19)
C9···H28"^{v}	3.08 (3)	H23′···H24	2.40 (3)
C10···H28"^{v}	3.05 (3)	H23′···C14^{vi}	2.76 (2)
C11···H22′^{v}	2.929 (19)	H23′···C15^{vi}	3.04 (2)
C14···H14^{x}	3.09 (2)	H24···H21	2.59 (3)
C14···H23′^{vi}	2.76 (2)	H24···H23′	2.40 (3)
C14···H20^{x}	3.02 (2)	H24′···S4	2.56 (2)
C15···H23′^{vi}	3.04 (2)	H25···H20	2.55 (3)
C17···H3^{iii}	2.95 (3)	H25′···H20′	2.47 (3)
C17···H9^{xi}	3.08 (2)	H28···C1^{vii}	3.09 (2)
C18···H7^{xi}	2.99 (2)	H28···C28^{ix}	3.02 (2)
C18···H22	2.809 (19)	H28···H28′^{ix}	2.57 (3)
C19···H22	2.77 (2)	H28′···C3^{ii}	2.96 (3)
C22···H18	3.08 (2)	H28′···C4^{ii}	3.09 (2)
C26···H15^{vi}	3.08 (2)	H28′···C28^{ix}	3.09 (2)
C28···H28^{ix}	3.02 (2)	H28′···H28^{ix}	2.57 (3)
C28···H28′^{ix}	3.09 (2)	H28"···C9^{vii}	3.08 (3)
H1···C8	3.07 (2)	H28"···C10^{vii}	3.05 (3)
H1···H7′	2.56 (4)	H28"···H9′^{vii}	2.55 (3)
H1···H8	2.57 (3)	H28"···H10′^{vii}	2.37 (4)
H3···C17^{iii}	2.95 (3)		

S1—Sn—S2	64.64 (1)	C8—C7—H7′	106.6 (15)
S1—Sn—S3	82.41 (1)	H7—C7—H7′	111 (2)
S1—Sn—S4	146.94 (1)	C7—C8—H8	108.0 (12)
S1—Sn—C27	103.06 (5)	C9—C8—H8	107.5 (11)
S1—Sn—C28	108.78 (5)	C12—C8—H8	108.3 (12)
S2—Sn—S3	146.97 (1)	C8—C9—H9	110.9 (12)
S2—Sn—S4	148.33 (1)	C8—C9—H9′	109.9 (12)
S2—Sn—C27	84.67 (5)	C10—C9—H9	106.6 (12)
S2—Sn—C28	82.01 (6)	C10—C9—H9′	108.7 (12)
S3—Sn—S4	64.71 (1)	H9—C9—H9′	107.8 (17)
S3—Sn—C27	106.16 (5)	N1—C10—H10	108.4 (12)
S3—Sn—C28	107.93 (6)	N1—C10—H10′	108.1 (11)
S4—Sn—C27	83.98 (6)	C9—C10—H10	110.6 (11)
S4—Sn—C28	85.70 (5)	C9—C10—H10′	110.9 (12)
C27—Sn—C28	135.64 (7)	H10—C10—H10′	108.5 (16)
Sn—S1—C13	94.81 (5)	N1—C11—H11	107.4 (12)
Sn—S2—C13	81.09 (6)	N1—C11—H11′	108.3 (12)
Sn—S3—C26	94.59 (5)	C12—C11—H11	108.4 (12)
Sn—S4—C26	81.01 (6)	C12—C11—H11′	109.7 (11)
C10—N1—C11	112.61 (14)	H11—C11—H11′	112.3 (16)
C10—N1—C13	123.18 (13)	C8—C12—H12	111.4 (13)
C11—N1—C13	123.85 (14)	C8—C12—H12′	108.9 (13)
C23—N2—C24	112.31 (13)	C11—C12—H12	109.1 (13)
C23—N2—C26	124.73 (14)	C11—C12—H12′	105.4 (13)
C24—N2—C26	122.86 (13)	H12—C12—H12′	110.5 (18)
C2—C1—C6	121.37 (18)	C15—C14—H14	119.8 (13)
C1—C2—C3	119.78 (19)	C19—C14—H14	119.4 (13)
C2—C3—C4	119.43 (19)	C14—C15—H15	117.1 (14)
C3—C4—C5	120.50 (19)	C16—C15—H15	122.9 (14)
C4—C5—C6	121.35 (19)	C15—C16—H16	120.5 (15)
C1—C6—C5	117.57 (18)	C17—C16—H16	119.5 (15)
C1—C6—C7	121.08 (16)	C16—C17—H17	120.0 (15)
C5—C6—C7	121.35 (18)	C18—C17—H17	120.1 (15)
C6—C7—C8	114.28 (15)	C17—C18—H18	120.1 (15)
C7—C8—C9	112.97 (13)	C19—C18—H18	118.7 (15)
C7—C8—C12	110.77 (14)	C19—C20—H20	109.4 (13)
C9—C8—C12	109.05 (14)	C19—C20—H20′	110.4 (12)
C8—C9—C10	112.83 (13)	C21—C20—H20	109.6 (12)
N1—C10—C9	110.23 (13)	C21—C20—H20′	107.9 (12)
N1—C11—C12	110.86 (14)	H20—C20—H20′	105.8 (17)
C8—C12—C11	111.47 (14)	C20—C21—H21	108.8 (12)
S1—C13—S2	118.74 (10)	C22—C21—H21	107.7 (12)
S1—C13—N1	118.28 (11)	C25—C21—H21	107.7 (11)
S2—C13—N1	122.98 (12)	C21—C22—H22	110.9 (11)
C15—C14—C19	120.82 (17)	C21—C22—H22′	109.6 (12)
C14—C15—C16	119.92 (19)	C23—C22—H22	106.9 (12)
C15—C16—C17	120.02 (19)	C23—C22—H22′	108.6 (12)
C16—C17—C18	119.9 (2)	H22—C22—H22′	108.4 (15)

C17—C18—C19	121.24 (18)	N2—C23—H23	109.2 (12)
C14—C19—C18	118.06 (16)	N2—C23—H23′	104.7 (13)
C14—C19—C20	121.05 (16)	C22—C23—H23	110.1 (12)
C18—C19—C20	120.85 (16)	C22—C23—H23′	111.1 (13)
C19—C20—C21	113.50 (15)	H23—C23—H23′	110.7 (17)
C20—C21—C22	112.28 (13)	N2—C24—H24	108.1 (12)
C20—C21—C25	110.50 (14)	N2—C24—H24′	109.8 (12)
C22—C21—C25	109.73 (13)	C25—C24—H24	109.9 (13)
C21—C22—C23	112.35 (13)	C25—C24—H24′	110.6 (13)
N2—C23—C22	110.82 (14)	H24—C24—H24′	108.6 (16)
N2—C24—C25	109.92 (14)	C21—C25—H25	111.0 (12)
C21—C25—C24	112.27 (14)	C21—C25—H25′	109.8 (12)
S3—C26—S4	118.58 (9)	C24—C25—H25	108.9 (12)
S3—C26—N2	118.22 (11)	C24—C25—H25′	107.5 (13)
S4—C26—N2	123.20 (12)	H25—C25—H25′	107.3 (17)
C2—C1—H1	121.2 (13)	Sn—C27—H27	106.8 (15)
C6—C1—H1	117.4 (13)	Sn—C27—H27′	107.0 (13)
C1—C2—H2	120.1 (15)	Sn—C27—H27"	107.2 (16)
C3—C2—H2	120.1 (15)	H27—C27—H27′	106 (2)
C2—C3—H3	121.1 (16)	H27—C27—H27"	119 (2)
C4—C3—H3	119.4 (16)	H27′—C27—H27"	110 (2)
C3—C4—H4	118.7 (19)	Sn—C28—H28	110.6 (17)
C5—C4—H4	120.8 (19)	Sn—C28—H28′	105.6 (16)
C4—C5—H5	119.7 (14)	Sn—C28—H28"	108.4 (17)
C6—C5—H5	118.8 (14)	H28—C28—H28′	110 (2)
C6—C7—H7	110.6 (12)	H28—C28—H28"	112 (3)
C6—C7—H7′	107.7 (18)	H28′—C28—H28"	110 (3)
C8—C7—H7	106.6 (12)		

S2—Sn—S1—C13	−4.91 (5)	C23—N2—C26—S3	−2.1 (2)
S3—Sn—S1—C13	177.56 (5)	C23—N2—C26—S4	178.30 (12)
S4—Sn—S1—C13	171.82 (5)	C24—N2—C26—S3	−177.99 (12)
C27—Sn—S1—C13	72.65 (7)	C24—N2—C26—S4	2.4 (2)
C28—Sn—S1—C13	−76.02 (8)	C6—C1—C2—C3	0.8 (3)
S1—Sn—S2—C13	5.14 (5)	C2—C1—C6—C5	−0.4 (3)
S3—Sn—S2—C13	9.63 (6)	C2—C1—C6—C7	178.65 (18)
S4—Sn—S2—C13	−171.46 (5)	C1—C2—C3—C4	−0.5 (3)
C27—Sn—S2—C13	−102.04 (7)	C2—C3—C4—C5	−0.2 (3)
C28—Sn—S2—C13	120.38 (7)	C3—C4—C5—C6	0.6 (3)
S1—Sn—S3—C26	−170.40 (5)	C4—C5—C6—C1	−0.3 (3)
S2—Sn—S3—C26	−174.50 (5)	C4—C5—C6—C7	−179.34 (18)
S4—Sn—S3—C26	6.13 (5)	C1—C6—C7—C8	−68.5 (2)
C27—Sn—S3—C26	−68.94 (8)	C5—C6—C7—C8	110.53 (19)
C28—Sn—S3—C26	82.24 (8)	C6—C7—C8—C9	−59.4 (2)
S1—Sn—S4—C26	−0.07 (6)	C6—C7—C8—C12	177.94 (15)
S2—Sn—S4—C26	174.28 (5)	C7—C8—C9—C10	−176.92 (15)
S3—Sn—S4—C26	−6.38 (5)	C12—C8—C9—C10	−53.29 (19)
C27—Sn—S4—C26	104.68 (7)	C7—C8—C12—C11	178.86 (15)

C28—Sn—S4—C26	−118.52 (7)	C9—C8—C12—C11	53.93 (18)
Sn—S1—C13—S2	8.94 (9)	C8—C9—C10—N1	54.50 (19)
Sn—S1—C13—N1	−170.60 (11)	N1—C11—C12—C8	−56.9 (2)
Sn—S2—C13—S1	−7.62 (8)	C19—C14—C15—C16	−0.6 (3)
Sn—S2—C13—N1	171.90 (13)	C15—C14—C19—C18	−0.4 (3)
Sn—S3—C26—S4	−11.09 (9)	C15—C14—C19—C20	177.23 (18)
Sn—S3—C26—N2	169.25 (12)	C14—C15—C16—C17	1.3 (3)
Sn—S4—C26—S3	9.49 (8)	C15—C16—C17—C18	−0.9 (3)
Sn—S4—C26—N2	−170.87 (14)	C16—C17—C18—C19	−0.2 (3)
C11—N1—C10—C9	−56.46 (18)	C17—C18—C19—C14	0.8 (3)
C13—N1—C10—C9	130.19 (16)	C17—C18—C19—C20	−176.87 (19)
C10—N1—C11—C12	58.24 (19)	C14—C19—C20—C21	−88.0 (2)
C13—N1—C11—C12	−128.46 (17)	C18—C19—C20—C21	89.6 (2)
C10—N1—C13—S1	−176.74 (12)	C19—C20—C21—C22	−57.05 (19)
C10—N1—C13—S2	3.8 (2)	C19—C20—C21—C25	−179.91 (13)
C11—N1—C13—S1	10.7 (2)	C20—C21—C22—C23	−174.71 (13)
C11—N1—C13—S2	−168.87 (12)	C25—C21—C22—C23	−51.41 (18)
C24—N2—C23—C22	−58.28 (17)	C20—C21—C25—C24	176.91 (14)
C26—N2—C23—C22	125.41 (16)	C22—C21—C25—C24	52.58 (18)
C23—N2—C24—C25	59.00 (17)	C21—C22—C23—N2	54.40 (17)
C26—N2—C24—C25	−124.62 (16)	N2—C24—C25—C21	−56.34 (18)

Symmetry codes: (i) $x-1, y+1, z$; (ii) $-x+1, -y+1, -z$; (iii) $-x+1, -y, -z$; (iv) $-x+3, -y+1, -z+1$; (v) $x-1, y, z$; (vi) $-x+3, -y, -z+1$; (vii) $x+1, y, z$; (viii) $x+1, y-1, z$; (ix) $-x+2, -y+1, -z$; (x) $-x+4, -y, -z+1$; (xi) $-x+2, -y, -z$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10···S2	0.98 (2)	2.54 (2)	3.0666 (19)	113.7 (14)
C11—H11′···S1	1.01 (2)	2.43 (2)	3.011 (2)	116.3 (14)
C23—H23···S3	0.94 (2)	2.490 (19)	3.0207 (18)	116.1 (14)
C24—H24′···S4	0.93 (2)	2.56 (2)	3.0681 (18)	114.9 (15)